Excitation energy dependence of the level density for fissionable nuclei

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Starting from a realistic set of single-particle levels, a microscopic calculation of nuclear level densities is performed. The washing out of the shells and the blocking of the pairing interaction with increasing excitation energy are shown for ^{240}Pu and ^{194}Hg at different deformations. For ^{210}Po the variation with the parameters of the nuclear potential is also discussed. Theoretical values at different deformations and excitation energies are compared with the existing experimental information on level density in ^{194}Hg, ^{193}Hg, ^{193}Au, and ^{190}Pt.

[NUCLEAR STRUCTURE, FISSION ^{194}Hg, ^{210}Po, ^{240}Pu; microscopic calculation of nuclear level densities; shell and pairing effects; dependence on excitation energy, deformation and nuclear parameters; comparison with experiment.]

I. FOREWORD

In the last decade, numerous studies of nuclear deexcitation following heavy-ion reactions have considerably increased the energy and angular momentum limits for which experimental evidence on level density can be obtained. This new experimental information, combined with rigorous calculations, can lead to a better understanding of the variation of the nuclear level density as a function of deformation, excitation energy, and angular momentum, and thus entirely justifies any new theoretical investigation of this problem.

In the rich literature on nuclear level densities,[1] two general attitudes in treating this subject stand out:

One is to fit the existing experimental data with simple analytical expressions[2,3] with a view to furnishing mass- and energy-independent parameters for subsequent statistical analyses of nuclear processes. Modified Bethe expressions have been employed allowing for shell and pairing effects and, recently,[4,5] also for the washing out of the shell effect with increasing excitation energy.

The other approach is to compare the spacing of the levels in a realistic model with the experimental level spacings for the final purpose—not yet attained—of deciding what kind of correlations should be included in the actual nuclear models to describe the high-energy spectra. But even in this approach one is sometimes tempted to arbitrarily adjust the model, e.g., the pairing strength,[6,7] in order to reproduce the experimental data.

In adopting the second attitude, two fundamentally different methods have been used to obtain the theoretical level density of a many-particle system.

Most often the level density is calculated by the Laplace inversion of the grand partition function.[6,8] This function can be evaluated only if the total energy of the system can be expressed as a sum of single-particle or -"quasiparticle" energies[9] and the method is essentially combinatorial. In this case the levels with a given spin and energy can also be directly counted,[7] and this arithmetical approach represents an excellent test for the more economical statistical mechanics approach.

The second method for obtaining the theoretical level density, insufficiently explored until now, is the so-called spectral distribution method.[10,11] It can take into account exactly any realistic residual interaction by exploiting gross properties of the distribution of levels for interacting particles in shell-model spaces with certain symmetries. The total level density is then obtained as a superposition of partial densities in these subspaces. The drawback of this method is that it can reproduce only general average trends of nuclei from a certain (Z, N) region, and not a peculiarity of a selected nucleus.

In the present paper, the results of the partition function method for ^{194}Hg and neighboring nuclei are compared with those extracted from the analyses of the slow-neutron resonances[3] and of the fission excitation function of ^{194}Hg produced in the reaction ^{182}W + ^{12}C (Ref. 12).

Before treating this particular case (Sec. IV), the formalism employed in obtaining the numerical results will be outlined (Sec. II) and checked for nuclei with well-known shell effects (Sec. III).

II. MODE OF CALCULATION

In statistical mechanics, nuclei can be described in terms of a generalized Gibbsian canonical ensemble of systems represented by points distri-

buted with a certain probability in the phase spaces. The normalization condition of this probability,

$$e^{\beta\Omega}\int\int \rho(E,A)\, e^{-\beta(E-\lambda A)}dE\, dA = 1\,, \quad \beta>0 \qquad (1)$$

is the basic relation for the evaluation of the nuclear level density $\rho(E,A)$; Ω is the generalized potential, λ is the chemical potential, β is the inverse of the temperature, and $\rho(E,A)$ is defined as the number of points which correspond to a given total energy E, in the phase space of A nucleons.

The level density can be obtained through the inversion of Eq. (1), regarded as a Laplace transform, if the generalized partition function $e^{-\beta\Omega}$ can be calculated.

For an infinitely large nucleus described by a pairing force Hamiltonian, this function assumes the following form[13,14]:

$$-\beta\Omega = -\beta\sum_{\alpha>0}(\epsilon_\alpha - \lambda - e_\alpha) + 2\sum_{\alpha>0}\ln[1+\exp(-\beta e_\alpha)] - \beta\Delta^2/|G|\,, \qquad (2)$$

if the generalized (for β finite) gap equation

$$2/|G| = \sum_{\alpha>0}\tanh(\tfrac{1}{2}\beta e_\alpha)/e_\alpha\,, \qquad (3)$$

which relates the gap parameter Δ to β and λ, is fulfilled. G is the pairing strength and e_α is the single-quasiparticle energy,

$$e_\alpha = [(\epsilon_\alpha - \lambda)^2 + \Delta^2]^{1/2}\,.$$

Of course, the formalism can be extended to nuclei with two different kinds of nucleons. The nuclear level density is then given by

$$\rho(E,N,Z) = \frac{1}{(2\pi i)^3}\int\int\int_{-i\infty}^{+i\infty}\exp[\beta(E-\Omega_N-\Omega_Z) - \alpha_N N - \alpha_Z Z] \times d\beta\, d\alpha_N\, d\alpha_Z\,, \qquad (4)$$

where $\alpha = \beta\lambda$. The triple integration can be performed, to a good approximation, by the saddle-point method. The application of this method to Eq. (4) was presented in detail in Appendix B of Ref. 15 and will not be repeated here.

When this formalism is used to describe finite nuclei, one should remember that it represents only a first-order approximation (the heavier the nucleus, the better the approximation), the accuracy of which is difficult to predict.

The total level density of a nucleus—seen as a $(Z+N)$ nucleon system—is then built on single proton and neutron energies ϵ_α, and is expected to depend strongly on the distribution of these energies [see also Eq. (5) below]. One should therefore choose the single-particle sets of levels as well as possible. In the present paper, the energies of a nucleon moving independently in a Cassinoidal-shape diffuse potential have been numerically obtained by the method described in Ref. 16. It can treat any nuclear shape appearing in symmetrical fission with only one deformation paramater ϵ. Besides, for the spherical case $\epsilon = 0$, the nuclear potential assumes the Woods-Saxon form. Thus, one can use the nuclear parameters already reported which most accurately reproduce the experimental single-particle and hole energies [in the (Z,N) region of interest] and which are the most suitable for our purpose. For the lead region, there are such parameters[17] and they have been employed in the present calculations. Of course, the direct use of the experimental single-particle spectra, when possible, is recommended.[18]

For a given excitation energy U, the usual Bethe expression

$$\rho(U) = \frac{1}{12}\left(\frac{\pi^2}{a}\right)^{1/4}\frac{1}{U^{5/4}}\exp[2(aU)^{1/2}] \qquad (5)$$

relates the many-particle level density ρ to the local (at the Fermi surface) single-particle level density $g_0 = (6a/\pi^2)$. Because of the shell effects, this average g_0 (or the related quantity a) of the density of levels with average occupation numbers n_α, different from one or zero, should vary both with deformation and with excitation energy. One can therefore treat a as a parameter and use Eq. (5) to fit the numerical results, obtained as described above.

The excitation energy is determined by

$$U = E(T = 1/\beta) - E(0)\,, \qquad (6)$$

where $E(0) = \sum_\alpha n_\alpha(0)\epsilon_\alpha$ is the true (shell-affected) ground state. There is no obvious reason to choose the liquid-drop energy as zero energy. The shells in the single-particle spectrum do not change substantially with nuclear temperature.[19] The shell structure is therefore preserved in highly excited nuclei; it is only less noticeable (i.e., "washed-out") since one averages over a wider energy interval. One can take, of course, any origin for U but only one is consistent with the interpretation of a as $(\pi^2/6)g_0$.

For highly deformed nuclei, the well-known monotonic increase of the shell-model total energy with deformation is unrealistic. Therefore, the validity of any equation containing shell-model energies should be questioned, e.g., Eqs. (2), (6), ...

To clear up this problem, a consistent Strutinsky-type renormalization of both E and Ω has been attempted.[20] The results show only a small change in the variation of the total level density with deformation, as compared to the unrenormalized results. Therefore the general conclusions of a traditional calculation, such as those discussed here, are still valid.

III. TYPICAL NUCLEI WITH STRONG SHELL EFFECTS: ^{240}Pu AND ^{210}Po

To follow more clearly the physics behind the variation of a with ϵ and U, and to provide an initial verification of the computational procedures used, two cases expected to exhibit strong variations of shell effects with deformation and nucleon number have been selected in this section.

In Fig. 1 are plotted the results for the main deformation states of ^{240}Pu: spherical shape ($\epsilon = 0.00$), ground state ($\epsilon = 0.21$), first saddle point ($\epsilon = 0.40$), second ground state ($\epsilon = 0.53$), and second saddle point ($\epsilon = 0.69$). The pairing interaction was neglected ($\Delta = 0$) in this example. The proportionality between g_0 and a at low excitation energy can be noticed.

There is a well-established connection between the local single-particle level density g_0 and the shell correction to the total energy.[21] One immediately notices it here: To (unstable) stable nuclear deformations always correspond (large) small values of the parameter a. As a consequence, in the energy region where the different curves are well separated, the shell effects are not completely washed out. At 100 MeV, for instance, the differences between the distributions of the single-particle energies at various ϵ are still readily noticeable, but it has often been stressed[22] that this result is related to the choice of zero energy in Eq. (6). In the so-called "back-shifted" Fermi-gas model, the excitation energy at high nuclear temperature is measured from the liquid-drop energy $E(0) - \delta_{\text{shell}}$, and in this case the curves of Fig. 1 bunch closer together (as indicated by the circles).

The back-shifted model is based on a supposed asymptotic behavior of the type[23]

$$\rho(U) \to \exp\{2[\tilde{a}(U + \delta_{\text{shell}})]^{1/2}\},$$

although it has not yet been possible to find the asymptotic parameters $\tilde{a}$ and δ_{shell}. The values one tries to extract always depend on the excitation energy U.[1,24,25]

As the relative distribution of the single-particle levels around the Fermi surface depends on ϵ, the washing out of the shells does not proceed identically for all deformations. This can be noticed more easily for the lower two curves which intersect (see also Fig. 5). Therefore a universal function $f(U)$, independent of N, Z, and ϵ, which reproduces this effect cannot be found, although it has been looked for in phenomenological approaches.[4] If such a function is considered to be indispensable, it should also include, as can be seen further on, the disappearance of the pairing interaction with U, which is quite another type of effect.

Figure 2 shows, for the same cases as in Fig. 1, the strong influence of the residual interactions on the level density: The appearance of the energy gap reduces considerably the number of levels in the low energy part of the spectrum. The effect is, of course, dependent on the value of the pair-

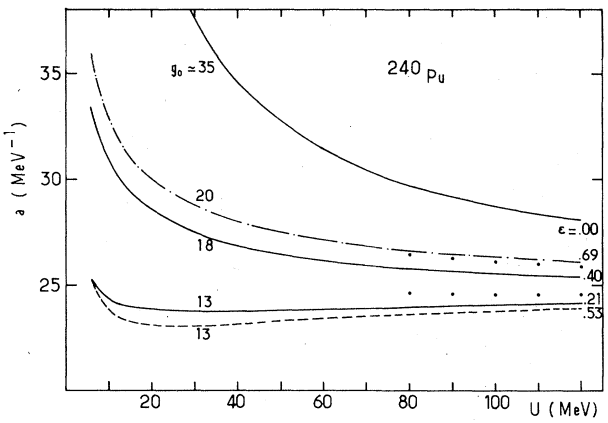

FIG. 1. Excitation energy dependence of the parameter a which fits the total level density for independent nucleons ($\Delta = 0$) in ^{240}Pu at different deformations, ϵ. g_0 is the number of levels per MeV, counted in the single-particle spectrum around the Fermi energy. The circles correspond to the choice of the liquid-drop energy as zero energy for $\epsilon = 0.00$ and $\epsilon = 0.53$.

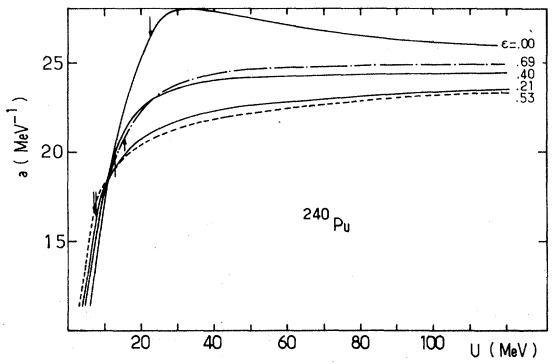

FIG. 2. The same as in Fig. 1, but with the inclusion of the pairing interaction between nucleons. The arrows indicate the excitation at which the pairing cancels.

ing strength G used,[15] but a more quantitative study is not attempted here.

With increasing excitation energy, the single-particle orbits eligible for mixing through pairing forces are gradually occupied by quasiparticles, which make them unavailable to the interacting pairs.[1,7] This blocking effect reduces both the depression of the ground state and the energy of the first excited state. In this way, at some critical excitation, the pairing vanishes.[26]

As discussed in the previous section, a dependence of the results on the set of single-particle levels, and implicitly on the parametrization of the nuclear potential, is expected. The overall trend of this dependence is easy to guess: The parameter a should diminish with the depth V_0, and grow both with the radius r_0, and with the diffuseness d. Consequently, the study of these variations presents no *a priori* interest, except to see to what extent the uncertainties in the nuclear parameters influence the resulting level densities. It is for this reason that such calculations have been performed for the ground state of ^{210}Po.

A detailed analysis (Fig. 3) reveals, however, a more complex influence of the nuclear parameters on the local density of the single-particle levels. At low excitation energies, a small variation of the nuclear parameters from their experimental values[17] always yields an increase of the parameter a, irrespective of the sense of the variation. Therefore, in the case of ^{210}Po, the hypersurface $a(V_0, r_0, d)$ has a local minimum for the real (ground-state) values of V_0, r_0, and d, just as it does for the collective deformations which define the stable nuclear shapes.[27] At high excitation energies, this minimum is washed out and the expected overall dependence of a with nuclear parameters is found.

In view of the close connection already mentioned between parameter a and nuclear stability, this result has a natural explanation. It is the consequence of a variational principle which determines the geometry of the average nuclear field by minimizing the total energy with respect to V_0 (Ref. 28), r_0, d, and deformation parameters, as in the Hartree-Fock method.

Since the results obtained from a fit to single-particle spectra by a phenomenological potential are consistent with those obtained from a variational principle, it proves that the Woods-Saxon parametrization used is realistic. It also suggests that, for the determination of nuclear parameters, simple phenomenological approaches could replace laborious self-consistent calculations.

In this section, the values of ϵ have been chosen in accordance with the provisions of Strutinsky's method[16] and correspond to zero excitation energy.

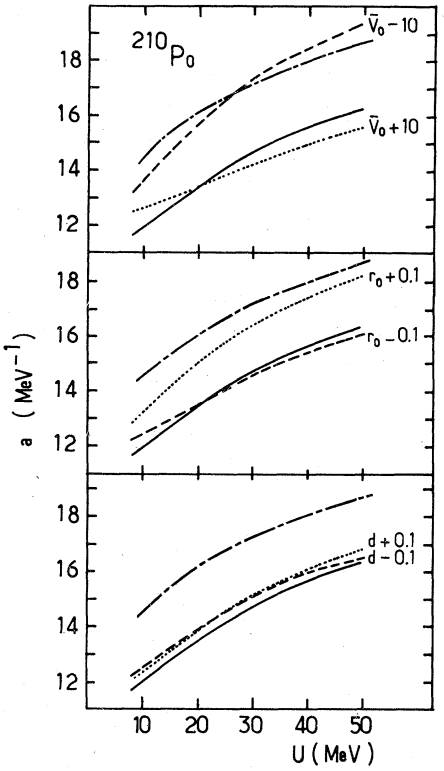

FIG. 3. Influence of the parametrization of the nuclear potential on the single-particle level density near the Fermi surface for the ground state ($\epsilon = 0.00$) of ^{210}Po. The solid curve corresponds to Woods-Saxon potential parameters which reproduce the experimental single-particle spectra in the lead region (Ref. 17): $V_0 = \bar{V}_0[1 \pm 0.862\,(N-Z)/A]$, $\bar{V}_0 = 49.65$ MeV, $r_0^{(p)} = 1.275$ fm, $r_0^{(n)} = 1.347$ fm, $d = 0.700$ fm. The dashed curves result from a decrease of the values of these parameters (one at a time) and the dotted curves from an increase of these values. The dot-dash curve corresponds to the two-center shell-model (Ref. 29).

Excited nuclei are in principle expected to be characterized by a distribution of deformation parameters rather than by a single value[15] and this changes the absolute value of their level density. However, the broadening of the distribution (as well as the shift of its most probable value towards zero), with increasing excitation energy, occurs at a rate inversely proportional to the magnitude of the shell effects involved[15]; hence, the level density at $\epsilon = 0$ still represents a good approximation of the actual level density for a strongly bound spherical nucleus and moderate excitation energies, as in Fig. 3. This is probably no longer true for ^{240}Pu at high excitation energies, but the above discussion on this case did not concern the absolute value of the density of nuclear levels.

On the contrary, for comparison to experiments (next section) we need absolute values of level

density that are as realistic as possible. Then the dependence of the nuclear shape on the excitation energy has to be taken into account.

IV. ^{194}Hg

Here, the experimental evidence on the density of levels in ^{194}Hg and in the products of its n, p, and α decay has also been used to test the validity of the formalism presented in Sec. II. Such evidence exists at about 7 MeV excitation energy for the ground-state deformation and at about 90 MeV for both ground-state and saddlepoint deformations. Data come from slow-neutron resonances[3] and from heavy-ion induced fission excitation functions,[12] respectively.

Figure 4 shows the oscillations of the single-particle level density with deformation at the Fermi surface of ^{194}Hg. In comparison with ^{240}Pu, they are less pronounced and shifted by about 0.1 towards smaller deformations. Since the liquid-drop fission barrier is, in turn, shifted by about 0.2 towards larger deformations,[30] the resulting shell-corrected barrier is almost single-humped and the ground state is slightly deformed. $\epsilon = 0.1$ was taken as the ground-state deformation of the four nuclei treated in this section: ^{194}Hg, ^{193}Hg, ^{193}Au, and ^{190}Pt.

In Table I, experimental and calculated (pure shell-model) values of the parameter a are given. The agreement is remarkably good for ground-state deformations and excitations equal to the neutron binding energies.

This shows that, in this region, the nuclei are deformed. (For a spherical shape the parameter a would have had to be 30% larger.) It also indicates that the critical energies at which the pairing cancels are close to the neutron binding energies. This last fact is supported to some extent by present calculations which predict critical excitations around 9 MeV for this nuclear region.

One should remember that the contribution of collective rotations[31] was not included in Table I. Hence, the good agreement with experiment apparently suggests that, in this nuclear region, such levels are not populated in slow-neutron capture reactions. However, one should be careful because a small missing contribution from rotational states could be compensated by the persistence of a weak pairing interaction.

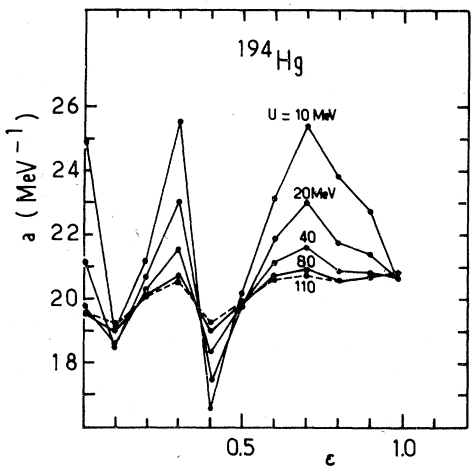

FIG. 4. Parameter a which fits the total level density for independent nucleons in ^{194}Hg at different deformations ϵ and excitation energies U. The calculated values are represented by closed circles.

At very high excitation energies the parameter a is nearly energy independent (Fig. 5). This justifies, *a posteriori*, the constant values generally used in the evaporation codes, but only at these energies. It also facilitates the comparison between theory and experiment since precise knowledge of the excitation energy is not necessary.

In Fig. 6 are plotted the calculated ratios a_f/a_n, a_α/a_n, and a_p/a_n • a_f corresponds to the liquid-drop saddle point for zero angular momentum: $\epsilon = 0.900$.[30] One could choose the saddle point for $J = 45\,\hbar$: $\epsilon = 0.800$,[32] or the shell-corrected saddle

TABLE I. Absolute and relative values of the level density parameter a for ^{194}Hg.

	From the fit of the slow-neutron resonance data (3), i.e., at $U \simeq 7$ MeV	From the fit of the calculated total level density for independent nucleons at $U = 6$ MeV	$U = 8$ MeV
$a_\gamma(^{194}\text{Hg})$	19.35	20.11	19.48
$a_n(^{193}\text{Hg})$	20.26	20.29	19.73
$a_p(^{193}\text{Au})$	21.05	21.77	20.91
$a_\alpha(^{190}\text{Pt})$	22.00	22.22	21.71
a_γ/a_n	0.96	0.99	0.99
a_p/a_n	1.04	1.07	1.06
a_α/a_n	1.09	1.10	1.10

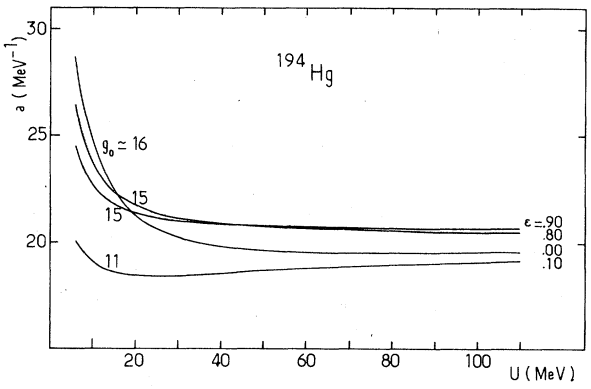

FIG. 5. The same as in Fig. 1, but for ^{194}Hg.

point: $\epsilon = 0.700$ (Fig. 4), but the differences are not significant in this energy domain (see Figs. 4 and 5).

With the values of a_α/a_n and a_p/a_n from slow-neutron resonances (first column of Table I), the best fit to the fission excitation function of ^{194}Hg, between 70 and 120 MeV, gives a ratio $a_f/a_n = 1.16$.[12] At very high excitation energies, the differences between neighboring nuclei are washed out and a_α/a_n and a_p/a_n tend towards one (see Fig. 6). With this limiting value, the same fit gives a ratio $a_f/a_n = 1.12$.[12]

If one assumes that all the incident energy is used to heat the compound nucleus, the present calculations predict a value $a_f/a_n \simeq 1.095$ [the average over the interval $E^* = 53-103$ MeV (Ref. 33) in Fig. 6]. But the temperature in the compound system does not reflect all this energy, since a good fraction of the incident energy is tied up in collective motions. One has to subtract 18 MeV, for instance, the rotational energy of ^{194}Hg at $J = 45\hbar$,[12] and this leads to a ratio $a_f/a_n \simeq 1.110$. Finally, this value has to be corrected for the modification of the ground-state nuclear shape with excitation energy. As mentioned in the previous section, one has to average over all possible deformation states. This can be done with the help of our Fig. 4 and of Fig. 14 from Ref. 15, where the deformation probabilities are given for ^{192}Pt at different excitation energies. In this way, one obtains a theoretical ratio $a_f/a_n = 1.065$ to be compared with the experimental values mentioned above. The difference of a few percent is probably due to more rotational levels at the saddle point than in the ground state. Unfortunately, at present, these levels cannot be counted at very high excitation energies.[8,31]

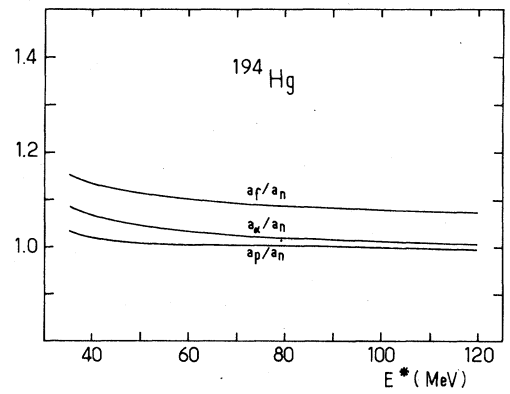

FIG. 6. Ratios between level density parameters versus excitation energy in the compound nucleus, ^{194}Hg, $E^* = U$ + fission barrier height (or particle binding energy).

V. SUMMARY AND CONCLUSIONS

The changes occurring in the density of levels with increasing excitation have been shown to be dependent on nuclear species and deformation. As a result, any phenomenological approach should be used with caution.

For ^{210}Po, the variation of the level density with the nuclear parameters was studied and a minimum of the level density parameter a was found for the experimental values of these parameters. This result suggests a consistency of the procedure and is worth studying in more detail.

In calculating nuclear level densities, critical assumptions are introduced only for the treatment of the residual interactions. If the critical excitation at which the pairing vanishes is exceeded, and if the basic set of single-particle levels is carefully chosen, the partition function approach seems to be a reliable method for the calculation of the total density of nuclear levels. Reasonably good agreement with relative and absolute level densities (extracted from different experimental data) was found for ^{194}Hg and neighboring nuclei, at different deformations and excitation energies. It appears that in this region of nuclei the contribution of the collective states is not very important.

To assess definitively the validity of the present approach, it should be applied also to other nuclei for which precise experimental information on level density can be obtained.

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